

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1612RXD

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS	9	FEB 08	STN Express, Version 8.3, now available
NEWS	10	FEB 20	PCI now available as a replacement to DPCI
NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/Caplus and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS EXPRESS		FEBRUARY 08	CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items
NEWS IPC8			For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 17:58:03 ON 07 APR 2008

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:58:25 ON 07 APR 2008

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STRUCTURE FILE UPDATES: 6 APR 2008 HIGHEST RN 1012582-98-7

DICTIONARY FILE UPDATES: 6 APR 2008 HIGHEST RN 1012582-98-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

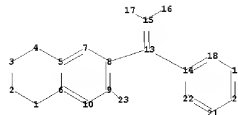
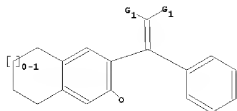
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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Uploading C:\Program Files\Stnexp\Queries\08141496.str



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ring nodes :
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ring bonds :
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20-21 21-22
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 9-23 15-16 15-17
exact bonds :
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normalized bonds :
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G1:C,H

Match level :

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10:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS

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L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 17:58:42 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 262 TO ITERATE

100.0% PROCESSED 262 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

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FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**

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PROJECTED ITERATIONS: 4269 TO 6211

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 17:58:48 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 5969 TO ITERATE

100.0% PROCESSED 5969 ITERATIONS
SEARCH TIME: 00.00.01

16 ANSWERS

L3 16 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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178.57

FILE 'CAPLUS' ENTERED AT 17:58:51 ON 07 APR 2008

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FILE COVERS 1907 - 7 Apr 2008 VOL 148 ISS 15

FILE LAST UPDATED: 6 Apr 2008 (20080406/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.

They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l3

L4 10 L3

=> d abs fbib hitstr 1-10

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

AB Retinoid X receptors (RXRs) play a crit. role in the regulation of many biol. activities and their specific agonists, including oxime ligands, functionally activate both homodimer RXR:RXR and heterodimer RXR:PPAR, the later relates to insulin sensitization and has a potential application in the treatment of type II diabetes. Based on RXR and 9-cis-RA complex crystallog. data, interaction between these compds. and RXR are simulated with DOCK 4.0. After minimizing each ligand-receptor complex, from resulting energy and activity an equation is deduced with the correlation coefficient $R^2 = 0.64$. Two CoMFA models are built and compared. One model originates from the ligand conformation extracted directly from complex, the other from energy-minimized ligands. The higher significance of the former than that of the later suggests that the conformation from induced fit of receptor be more reliable.

AN 2001:895932 CAPLUS Full-text

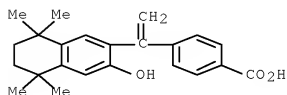
DN 136:177481

TI Molecular modeling and QSAR studies on the interaction mechanism of retinoids binding to RXR

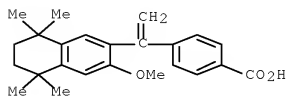
AU Guo, Zong-Ru; Yi, Xiang; Wang, Min-Min; Chu, Feng-Ming

CS Institute of Materia Medica, Peking Union Medical College, Chinese Academy

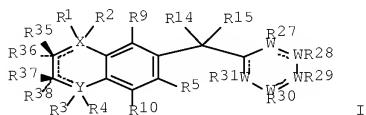
of Medical Sciences, Beijing, 100050, Peop. Rep. China
 SO Huaxue Xuebao (2001), 59(11), 1925-1931
 CODEN: HHHPA4; ISSN: 0567-7351
 PB Kexue Chubanshe
 DT Journal
 LA Chinese
 IT 153559-58-1 158499-05-9
 RL: PAC (Pharmacological activity); BIOL (Biological study)
 (mol. modeling and QSAR studies on interaction mechanism of retinoids
 binding to RXR)
 RN 153559-58-1 CAPLUS
 CN Benzoic acid, 4-[1-(5,6,7,8-tetrahydro-3-hydroxy-5,5,8,8-tetramethyl-2-
 naphthalenyl)ethenyl]- (CA INDEX NAME)



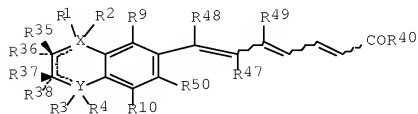
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 naphthalenyl)ethenyl]- (CA INDEX NAME)



L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
 GI



I



II

AB Title compds. (I, II, etc.; R1-R4 = H, alkyl, aralkyl, heteroarylalkyl; R5 = alkyl, heteroalkyl, aryl, heteroaryl, aralkyl, heteroaralkyl, amino, alkoxy, etc.; R14, R15 = H, alkyl, acyl, OH, alkoxy; R14R15 = O, (substituted) methano, oxime, hydrazone, epoxy, 1,3-dioxolanyl, 1,3-dioxanyl, 1,3-dithiolanyl, 1,3-dithianyl, oxazolidinyl, etc.; R27-R31 = H, alkyl, heteroalkyl, halo, amino, NO2, OH, alkoxy, etc.; R35-R38 = H, alkyl, OH, alkoxy; R35R36 or R37R38 = keto, or R35R36, R37R38, R35R37, or R36R38 = epoxy; R40 = OH, alkoxy, aralkoxy, heteroaralkoxy, amino; X, Y = C, O, S, N, SO, SO2; W = C, N, S, O; R47 = H, alkyl; R48, R49 = alkyl; R50 = alkyl, heteroalkyl, aryl, heteroaryl, aralkyl, heteroaralkyl, amino, alkoxy, etc.), were prepared Thus, 3-n-propyl-5,6,7,8-tetrahydro-5,5,8,8- tetramethylnaphthalene and monomethyl terephthalate acid chloride in CH2Cl2 were treated with AlCl3 to give after ester hydrolysis 4-[(3-n-propyl-5,5,8,8-tetramethyl-5,6,7,8-tetrahydro-2- naphthyl)carbonyl]benzoic acid (III). Title compds. showed antagonist potencies of IC50 = 5-673 nM in a screen using RXRa receptors and LGD1069 as agonist. Capsules, tablets, suppositories, and i.v. dosage forms containing III are given.

AN 1997:361549 CAPLUS Full-text
DN 126:330501

TI Preparation of naphthylcarbonylbenzoates, naphthylmethyloctatrienoates, and related compounds as dimer-selective retinoid X receptor modulators.

IN Canan-Koch, Stacie; Hwang, Chan Kou; Boehm, Marcus F.; Badea, Beth Ann; Dardashti, Laura J.; Zhang, Lin; Nadzan, Alex M.; Heyman, Richard A.; Mukherjee, Ranjan; Lala, Deepak S.; Farmer, Luc J.; et al.

PA Ligand Pharmaceuticals Incorporated, USA

SO PCT Int. Appl., 181 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 3

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PATENT FAMILY INFORMATION:

FAN 1997:290542

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OS MARPAT 126:330501

IT 189697-50-5F 189697-55-0F 189697-59-4F
189698-07-5F

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

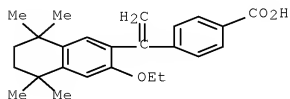
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and

related compds. as dimer-selective retinoid X receptor modulators)

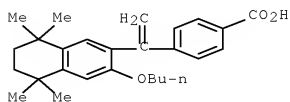
RN 189697-50-5 CAPLUS

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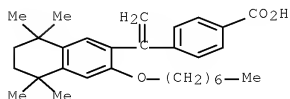
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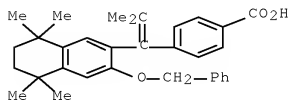
RN 189697-59-4 CAPLUS

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RN 189698-07-5 CAPLUS

CN Benzoic acid, 4-[2-methyl-1-[5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-3-(phenylmethoxy)-2-naphthalenyl]-1-propenyl]- (9CI) (CA INDEX NAME)



IT 189698-26-8F 189699-09-0F

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

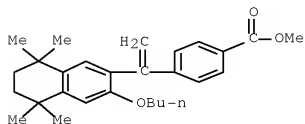
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and

related compds. as dimer-selective retinoid X receptor modulators)

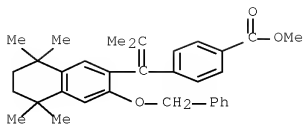
RN 189698-26-8 CAPLUS

CN Benzoic acid, 4-[1-(3-butoxy-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)ethenyl]-, methyl ester (CA INDEX NAME)

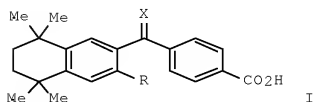


RN 189699-09-0 CAPLUS

CN Benzoic acid, 4-[2-methyl-1-[5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-3-(phenylmethoxy)-2-naphthalenyl]-1-propenyl]-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
GI



AB Two series of potent retinoid X receptor (RXR)-selective compds. were designed and synthesized based upon recent observation that (E)-4-[2-(5,5,8,8-tetramethyl-5,6,7,8-tetrahydro-2-naphthalenyl)-1-propenyl]benzoic acid binds and transactivates only the retinoic acid receptor (RAR) subtypes whereas its 3-Me derivative binds and transactivates both the RAR and RXR subfamilies. Functional groups in the 3-position of the tetrahydronaphthalenes I [R = H, alkyl, halo, OH, OMe; X = O, CH₂] results in compds. which elicit potent and selective activation of the RXR class. Such RXR-selective compds. offer pharmacol. tools for elucidating the biol. role of the individual retinoid receptors with which they interact. Activation profiles in cotransfection and competitive binding assays as well as mol. modeling calcs. demonstrate critical structural determinants that confer selectivity for members of the RXR subfamily. The most potent compound of these series, I [R = Me, X = CH₂], is the first RXR-selective retinoid (designated as LGD1069) to enter clin. trials for cancer indications.

AN 1994:656056 CAPLUS Full-text
DN 121:256056

TI Synthesis and Structure-Activity Relationships of Novel Retinoid X Receptor-Selective Retinoids

AU Boehm, Marcus F.; Zhang, Lin; Badea, Beth Ann; White, Steven K.; Mais, Dale E.; Berger, Elaine; Suto, Carla M.; Goldman, Mark E.; Heyman, Richard A.

CS Department of Medicinal Chemistry, Ligand Pharmaceuticals Inc., San Diego, CA, 92121, USA

SO Journal of Medicinal Chemistry (1994), 37(18), 2930-41
CODEN: JMCMAR; ISSN: 0022-2623

DT Journal
LA English

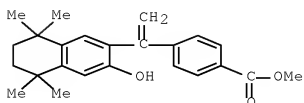
IT 158499-12-8P 158499-13-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of
tetrahydronaphthylethenylbenzoic
acids)

RN 158499-12-8 CAPLUS

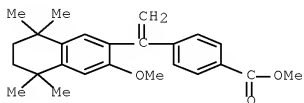
CN Benzoic acid, 4-[1-(5,6,7,8-tetrahydro-3-hydroxy-5,5,8,8-tetramethyl-2-

naphthalenyl)ethenyl]-, methyl ester (CA INDEX NAME)



RN 158499-13-9 CAPLUS

CN Benzoic acid, 4-[1-(5,6,7,8-tetrahydro-3-methoxy-5,5,8,8-tetramethyl-2-naphthalenyl)ethenyl]-, methyl ester (CA INDEX NAME)

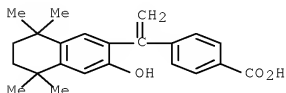


IT 153559-58-1P 158499-05-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and retinoid receptor binding of)

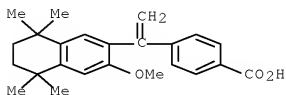
RN 153559-58-1 CAPLUS

CN Benzoic acid, 4-[1-(5,6,7,8-tetrahydro-3-hydroxy-5,5,8,8-tetramethyl-2-naphthalenyl)ethenyl]- (CA INDEX NAME)



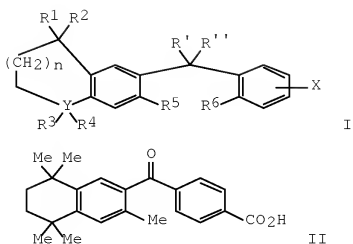
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CN Benzoic acid, 4-[1-(5,6,7,8-tetrahydro-3-methoxy-5,5,8,8-tetramethyl-2-naphthalenyl)ethenyl]- (CA INDEX NAME)



L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

GI



AB Ligands which selectively activate retinoid X receptors (RXR) in preference to retinoic acid receptors (RAR) are claimed. Claimed per se are several Markush structures, e.g., compds. I [R1, R2 = H, alkyl, acyl; Y = C, O, S, N, CH(OH), CO, SO, SO2, or a salt derivative; R3, R4 = H, alkyl, or is absent; R', R'' = H, alkyl, acyl, OH, alkoxy, thiol, thio ether, amino; or R'R'' = :O, :CH2, :S, :NOH, :NCN, CH2CH2, CH2O, etc.; R5, R6 = H, alkyl, halo, NO2, OH, alkoxy, SH, alkylthio, (di)(alkyl)amino, etc.; X = CO2H or derivs., CHO, tetrazolyl, PO3H2, SO3H, CH2OH, etc.], represented by 43 synthetic examples. Thus, acylation of 1,1,4,4,6-pentamethyl- 1,2,3,4-tetrahydronaphthalene by mono-Me terephthalate using PC15 and then AlCl3, and saponification of the ester product, gave title compound II. In a cotransfection assay, II activated RXR subtypes (α , β , γ) with efficacies of 130%, 52%, and 82%, resp. (vs. all-trans-retinoic acid as 100%), but had <2% to <4% efficacy for RAR subtypes. I synergistically increased the activities (e.g., antihyperproliferative) of RAR-active ligands, as well as other hormonal systems (e.g., clofibrate and 1,25-dihydroxyvitamin D activities).

AN 1994:217004 CAPLUS Full-text

DN 120:217004

TI Compounds (naphthalene and indane derivatives) having selectivity for retinoid X receptors

IN Boehm, Marcus F.; Heyman, Richard A.; Zhi, Lin

PA Ligand Pharmaceuticals Inc., USA

SO PCT Int. Appl., 101 pp.

CODEN: PIXXD2

DT Patent

LA English

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ES 2129115	T3	19990601	ES 1994-902184		19931022
			US 1993-3223	A	19930111
			US 1993-27747	A	19930305
			US 1993-52050	A	19930421
AT 187434	T	19991215	AT 1994-901195		19931022
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			US 1993-52051	A	19930421
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			US 1993-27747	A	19930305
			US 1993-52051	A	19930421
			WO 1993-US10204	W	19931022
PT 678086	T	20000531	PT 1994-901195		19931022
			US 1993-3223	A	19930111
			US 1993-27747	A	19930305
			US 1993-52051	A	19930421
NO 9403943	A	19941221	NO 1994-3943		19941018
			US 1992-872707	A	19920422

			US 1992-944783	A	19920911
			US 1993-3223	A	19930111
			US 1993-27747	A	19930305
			US 1993-52051	A	19930421
			WO 1993-US3944	A	19930422
US 5780676	A	19980714	US 1995-485386		19950607
			US 1992-872707	B2	19920422
			US 1992-944783	B2	19920911
			US 1993-3223	B2	19930111
			US 1993-27747	B2	19930305
			US 1993-52050	B2	19930421
			US 1993-141246	A1	19931022
US 5962731	A	19991005	US 1995-472784		19950607
			US 1992-872707	B2	19920422
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			US 1993-3223	B2	19930111
			US 1993-27747	B2	19930305
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US 6043279	A	20000328	US 1997-799396		19970212
			US 1992-872707	B2	19920422
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US 6610883	B1	20030826	US 1998-115615		19980713
			US 1992-872707	B2	19920422
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US 6320074	B1	20011120	US 1998-179674		19981027
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			US 1993-3223	A	19930111
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GR 3034841	T3	20010228	GR 2000-402529		20001113
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			US 1993-52051	A	19930421
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US 20060106072	A1	20060518	US 2005-300039		20051213
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			US 1992-944783	B2	19920911
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US 1993-52051
US 1993-141496

B2 19930421
A1 19931022

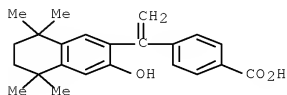
OS MARPAT 120:217004

IT 153559-58-1F

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as retinoid receptor ligand)

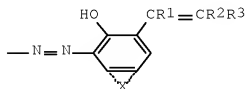
RN 153559-58-1 CAPLUS

CN Benzoic acid, 4-[1-(5,6,7,8-tetrahydro-3-hydroxy-5,5,8,8-tetramethyl-2-naphthalenyl)ethenyl]- (CA INDEX NAME)



L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

GI



I

AB An electrophotog. photoconductor has on an electroconductive support a photosensitive layer containing a charge-generating azo pigment having a structure in which a substituted or unsubstituted aromatic hydrocarbon or aromatic heterocyclic ring is bonded to an organic residue I (R1, R2 = H, alkyl, acyl, aryl, aralkyl, cyano; R3 = aromatic hydrocarbon or heterocyclic group containing optional substituents; X = organic residue forming polycyclic aromatic ring or heterocycle by fusion with the benzene ring) directly or via a linking group.

AN 1990:506321 CAPLUS [Full-text](#)

DN 113:106321

TI Electrophotographic photoconductor containing azo pigment

IN Kashizaki, Yoshiro

PA Canon K. K., Japan

SO Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 01100560	A	19890418	JP 1987-257377	19871014
	JP 08014703	B	19960214		
				JP 1987-257377	19871014

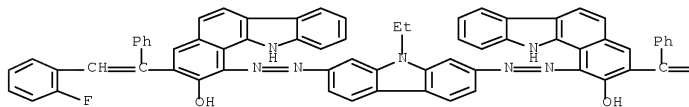
IT 126610-24-4F 126646-70-6F

RL: SPN (Synthetic preparation); PREP (Preparation)

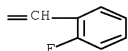
(preparation and use of, as electrophotog. charge-generating agent)

RN 126620-24-4 CAPLUS
 CN 11H-Benzo[a]carbazol-2-ol, 1,1'-[(9-ethyl-9H-carbazole-2,7-diyl)bis(azo)]bis[3-[2-(2-fluorophenyl)-1-phenylethenyl]- (9CI) (CA INDEX NAME)

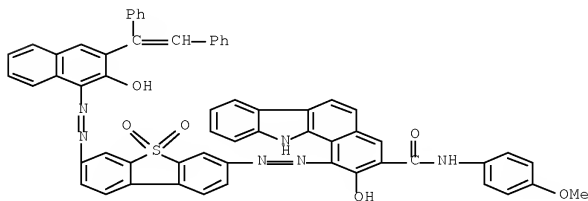
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PAGE 1-B

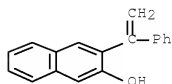


RN 126646-70-6 CAPLUS
 CN 11H-Benzo[a]carbazole-3-carboxamide, 1-[[[7-[[3-(1,2-diphenylethenyl)-2-hydroxy-1-naphthalenyl]azo]-5,5-dioxido-3-dibenzothienyl]azo]-2-hydroxy-N-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

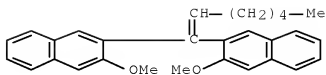


L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
 AB Ketones reacted with aluminum phenoxides in refluxing xylene to give 56-91% isomerically pure o-vinyl phenols. E.g., Al(OPh)₃, generated in situ from PhOH and Al turnings, reacted with Me₂CO (20 h) to give 56% 2-CH₂:CMeC₆H₄OH.
 AN 1980:58353 CAPLUS Full-text
 DN 92:58353
 OREF 92:9659a,9662a
 TI Regiospecificity in reactions between metal phenoxides and ketones. One-step synthesis of ortho-vinylphenols
 AU Casiraghi, Giovanni; Casnati, Giuseppe; Sartori, Giovanni; Bolzoni, Luciana

CS Ist. Chim. Org., Univ. Parma, Parma, Italy
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and
 Bio-Organic Chemistry (1972-1999) (1979), (8), 2027-9
 CODEN: JCPRB4; ISSN: 0300-922X
 DT Journal
 LA English
 OS CASREACT 92:58353
 IT 72471-04-6
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by reaction of aluminum phenoxide with ketone)
 RN 72471-04-6 CAPLUS
 CN 2-Naphthalenol, 3-(1-phenylethenyl)- (CA INDEX NAME)



L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
 GI For diagram(s), see printed CA Issue.
 AB Long-chain alkyl substitution at positions 5, 6, and 8 of 1,3-diaminobenzo[f]quinazoline derivs. (folate antagonist) did not affect or decrease the antibacterial and cytotoxic action compared to that of the parent compds., but increased the antimalarial activity. The most active compound against Plasmodium berghei in mice was 1,3-diamino-6-n-hexylbenzo[f]quinazoline (I) [53526-04-8], which at 640 mg/kg s.c.increased survival time almost 3-fold compared to controls. The most potent antibacterial activity in vitro was shown by 1,3-diamino-6-chlorobenzo[f]quinazoline [53526-05-9] against Streptococcus faecium (50% inhibitory dose 0.003 µM). I was prepared by reaction of 1-bromonaphthalene [90-11-9] with n-hexyllithium [1934-75-4], nitration in the free position, catalytic hydrogenation to the amine, and reaction with Na dicyanamide.
 AN 1975:508137 CAPLUS Full-text
 DN 83:108137
 OREF 83:16881a,16884a
 TI Quinazolines. 12. 1,3-Diaminobenzo[f]quinazolines containing long-chain alkyl or chloro substituents on the central ring. Synthesis and biological evaluation as candidate antifolate and antimalarial agents
 AU Rosowsky, Andre; Huang, Ping C.; Papatathanasopoulos, Nickolas; Modest, Edward J.
 CS Child. Cancer Res. Found., Harvard Med. Sch., Boston, MA, USA
 SO Journal of Medicinal Chemistry (1974), 17(11), 1217-22
 CODEN: JMCMAR; ISSN: 0022-2623
 DT Journal
 LA English
 IT 53526-16-2
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reduction of)
 RN 53526-16-2 CAPLUS
 CN Naphthalene, 2,2'-(1-heptenyldiene)bis[3-methoxy- (CA INDEX NAME)



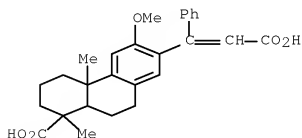
L4 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

AB A method is given for the prepn. of intermediates for the synthesis of aldosterone and 18-hydroxycorticosterone. EtMgBr (from Mg 2.432 and EtBr 9.820) in anhydrous Et2O 110 is cooled to 12-15°, freshly distilled ethoxyacetylene 7.88 in anhydrous Et2O 51.5 added over 30 min., when ethane ceases to evolve the mixture stirred 15 min. with ice H2O cooling, the system homogenized by addition of C6H6 110, 2 → 4β-lactone of 2α-methallyl-2β-carboxy-4bβ-methyl-7,7-ethylenedioxy- 1,2,3,4,4aα,4b,5,6,7,8,10,10aβ-dodecahydrophenanthren-4β- ol-1-one 7.115 in C6H6 80 parts added dropwise over 15 min. at 0-3°, the mixture stirred 3 hrs. at this temperature, ice and saturated NH4Cl added, the organic layer washed with NH4Cl solution and H2O, dried, filtered, evaporated in vacuo, the residue dissolved in Et2O, filtered through activated C, and concentrated to give 2 → 4β-lactone of 1-ethoxyethynyl- 2α-methallyl-2β-carboxy-4bβ-methyl-7,7-ethylenedioxy-1,2,3,4,4aα,4b,5,6,7,8,10,10aβ-dodecahydrophenanthrene-1,4β-diol (I), m. 138-40°. I 221.3 in anhydrous C5H5N 6500 is agitated with 10% Pd-CaCO3 100 parts at room temperature in H atmospheric, after 1 mole H is absorbed the mixture filtered, the residue washed with C5H5N, the filtrate evaporated to dryness in vacuo, the residue dissolved in Et2O, filtered through activated C, concentrated to a small volume, and cautiously mixed with petr. ether to give 2 → 4β-lactone of 1-ethoxyvinyl-2α-methallyl-2β-carboxy-4bβ-methyl-7,7-ethylenedioxy-1,2,3,4,4aα,4b,5,6,7,8,10,10aβ- dodecahydrophenanthrene-1,4β-diol (II), m. 18.5-110° and 136-7°. To II 4.45 in anhydrous C5H5N 200 under anhydrous N atmospheric is added dropwise 2M SOCl2 55 in anhydrous C5H5N at 0-3° over 5 min., the mixture stirred an addnl. 15 min. at this temperature, poured into M NH4HCO3 1000 and ice 100, the vessel washed with Et2O 1250 parts, after thorough agitation the ether solution washed with ice-cold M NH4HCO3 and ice H2O, dried, filtered, distilled in vacuo, and the residue recrystd. from Et2O to give 2 → 4β-lactone of 1,1-formylmethylene-2-αmethallyl- 2β-carboxy-4bβ-methyl-7,7-ethylenedioxy-1,2,3,4,4aα,4b,5,6,7,8,10,10aβ-dodecahydrophenanthren-4β- ol (III), m. 188-90°. III 39.85 in anhydrous EtOH 1000 is mixed with 2.5% Pd-SrCO3 10 parts at room temperature under H, after 0.95 mole equivalent H is absorbed the solution filtered, the filtrate evaporated in vacuo, the mixture fractionated on a cellulose column in 80% aqueous MeOH-heptane, and the product recrystd. from Et2O-petr. ether to give 2 → 4β-lactone of 1β-formylmethyl-2α-methallyl-2β-carboxy-4bβ-methyl- 7,7-ethylenedioxy-1,2,3,4,4aα,4b,5,6,7,8,10,10aβ-dodecahydrophenanthren-4β-ol (IV). IV 4.005 in C6H6 50 is mixed with OsO4 2.670, the mixture stirred 3 hrs. under N, MeOH 350 added, the solution mixed with Na2SO3 6.3 in H2O 100, agitated 20 min. under N, filtered, the filtrate freed of organic solvents in vacuo, the aqueous suspension extracted with CH2Cl2, the exts. washed with icecold N Na2CO3 and H2O, dried, evaporated, the product dissolved in MeOH 89 and C5H5N 1, paraperiodic acid 3.4 in H2O 10 parts added, the mixture stirred 1 hr. at room temperature under N, diluted with H2O, extracted with 3:1 Et2O-CH2Cl2, the exts. washed with H2O, dried, and evaporated in vacuo to give 2 → 4β-lactone of 1β-formylmethyl- 2α-acetonyl-2β-carboxy-4bβ-methyl-7,7-ethylenedioxy-1,2,3,4,4aα,4b,5,6,7,8,10,10aβ-dodecahydrophenanthren-4β- ol. Prepared similarly are: 2 → 4β-lactone of 1-ethoxyethynyl-2α-allyl-2β-carboxy-4bβ-

methyl-7,7- ethylenedioxy-1,2,3,4,4aa,4b,5,6,7,8,10,10aβdodecahydrophenanthrene-1,4β-diol, m. 149-52°; 2 → 4β-lactone of 1-(2-ethoxyvinyl)-2α-allyl-2β-carboxy-4bβ-methyl-7,7- ethylenedioxy-1,2,3,4,4aa,4b,5,6,7,8,10,10aβ-dodecahydrophenanthrene-1,4β-diol, m. 120-2°; 2 → 4β-lactone of 1β-formylmethyl-2α-allyl-2β-carboxy- 4bβ-methyl-7,7-ethylenedioxy-1,2,3,4,4aa,4ab,5,6,7,8,10,10a.bet a.-dodecahydrophenanthren-4β-ol; 2 → 4β-lactone of 1β,2α-bis (formylmethyl)-2β-carboxy-4bβ-methyl-7,7- ethylenedioxy-1,2,3,4.4aa,4b,5,6,7,8,10,10aβ- dodecahydrophenanthren-4β-ol; and 2 → 4β-lactone of 1β-formylmethyl-2α-(ω-acetoxyacetonyl)-2β-carboxy- 4bβ-methyl-7,7-ethylenedioxy-1,2,3,4,4aa,4b,5,6,7,8,10,10a.beta .-dodecahydrophenanthren-4β-ol.

AN 1961:87417 CAPLUS Full-text
 DN 55:87417
 OREF 55:16506i,16507a-h
 TI Polyhydrophenanthrene compounds
 IN Reichstein, Tadeus
 DT Patent
 LA Unavailable
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 805606		19581210	GB 1957-78257	19550114
IT	103033-89-2				
	(Derived from data in the 6th Collective Formula Index (1957-1961))				
RN	103033-89-2	CAPLUS			
CN	2-Phenanthreneacrylic acid, 8-carboxy-4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-4b,8-dimethyl-β-phenyl- (6CI) (CA INDEX NAME)				



L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
 AB Me O-methyl-7-acetylpodocarpate (Ia) 1500 and BrCH₂CO₂Et 770 in C₆H₆ 2640 added with heating to specially prepared Zn 313 parts, the mixture refluxed 2 hrs., unreacted Zn removed, and the mixture acidified gave Me O-methyl-7-[2-(1-ethoxycarbonyl-2-hydroxypropyl)]podocarpate (I), b₀.07 190-7°, [α]_D 105°. I 1500, AcCl 1650, and Ac₂O 2300 parts refluxed 50 min. gave Me O-methyl-7-(α-methyl-β-ethoxycarbonylvinyl)podocarpate (II), b₀.15 195°, [α]_D 117°. The β-MeO analog was similarly obtained by substitution of Me bromoacetate. II 288, KOH 100, propylene glycol 2100, H₂O 500, and MeOH 320 parts heated 3 hrs. at 90-100° gave Me O-methyl-7-(α-methyl-β-carboxyvinyl)podocarpate (III). [α]_D 129°. I 200, H₂O 2000, MeOH 3200, and NaOH 300 parts refluxed 4 hrs. gave Me O-methyl-7-[2-(1-carboxy-2-hydroxypropyl)]podocarpate. III heated 1.5 hrs. at 210° with C₅H₅N.HCl gave the lactone of 7-(α-methyl-β-carboxyvinyl)podocarpic acid, m. 287-9° (MeOH). Me O-methylpodocarpate and PhCl at 10° treated 10 min. with AlCl₃, the mixture stirred 3 hrs. at 10° with EtCOCl in PhCl, left 15 hrs. at room temperature, decomposed, the PhCl steam distilled, and the solid recrystd. gave Me O-methyl-7-propionylpodocarpate

(IV), m. 100-2° (MeOH). IV in C6H6 treated as above with BrCH2CO2Et and Zn dust gave after acetylating, Me O-methyl-7-(α -ethyl- β -ethoxycarbonylvinyl)podocarpate (V), b0.01 185-95°. V, KOH, MeOH, H2O, and propylene glycol heated 3 hrs. gave Me O-methyl-7-(α -ethyl- β -carboxyvinyl)podocarpate. Ia and MeCHBrCO2Et in C6H6 treated with Zn and the mixture refluxed 2 hrs. gave Me O-methyl-7-[2-(2-hydroxy-3-ethoxycarbonylbutyl)podocarpate (VI), b0.08 200°. VI, AcCl, and Ac2O refluxed 1 hr. and distilled gave Me O-methyl-7-(α , β -dimethyl- β -ethoxycarbonylvinyl)podocarpate (VII), b0.1 190°. VII 100, KOH 35, propylene glycol 720, H2O 180, and MeOH 100 parts heated 3 hrs. at 90-100° gave Me O-methyl-7-(α , β -dimethyl- β -carboxyvinyl)podocarpate. Et2SO4 refluxed 5 min. with podocarpic acid and NaOH in 50% alc. gave Et O-ethylpodocarpate (VIII). VIII treated with AcCl, PhNO2, and AlCl3 3 hrs. at 0° and left 100 hrs. gave Et O-ethyl-7-acetylpodocarpate (IX). IX treated with Et 2-bromohexanoate and the product dehydrated and hydrolyzed gave Et O-ethyl-7-(α -methyl- α -butyl- β -carboxyvinyl)podocarpate, [α]D 106°. Me O-methylpodocarpate treated 18 hrs. at 25° with AlCl3, BzCl, and PhCl gave Me O-methyl-7-benzoylpodocarpate, m. 114-19°. This material converted into Me O-methyl-7-(α -phenyl- β -ethoxycarbonylvinyl)podocarpate (X), m. 163-5.5°. X heated 1.5 hrs. at 210° with C5H5N.HCl gave the lactone of 7-(α -phenyl- β -carboxyvinyl)-podocarpic acid (XI), m. 242-5°. XI in MeOH left 0.5 hr. with Et2SO4 and Na2CO3 gave the lactone of Et 7-(α -phenyl- β -carboxyvinyl)podocarpate. X in H2O autoclaved 8 hrs. at 150° with alc. and KOH gave O-methyl-7-(α -phenyl- β -carboxyvinyl)podocarpic acid (XII). XII and C5H5N.HCl heated 10 min. at 210° and the product chromatographed on silica gel gave lactone of Me 7-(α -methyl- β -carboxyvinyl)podocarpate, m. 267-9° (CHCl3-MeOH). V in C5H5N.HCl heated 1.5 hrs. at 210° gave lactone of 7-(α -ethyl- β -carboxyvinyl)podocarpic acid.

AN 1961:87416 CAPLUS [Full-text](#)

DN 55:87416

OREF 55:16506c-i

TI 1,12-Dimethyl-6-hydroxy-7-(β -carboxyalkenyl)-1,2,3,4,9,10,11,12-octahydrophenanthrene-I-carboxylic acid esters

IN Bible, Roy H., Jr.

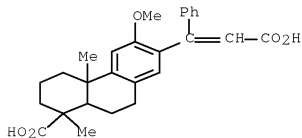
PA G.D. Searle and Co.

DT Patent

LA Unavailable

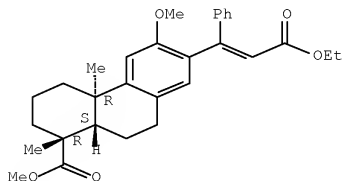
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2971008		19600000	US	
IT	103033-89-2	124422-36-2			
	(Derived from data in the 6th Collective Formula Index (1957-1961))				
RN	103033-89-2	CAPLUS			
CN	2-Phenanthreneacrylic acid, 8-carboxy-4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-4b,8-dimethyl- β -phenyl- (6CI) (CA INDEX NAME)				



RN 124422-36-2 CAPLUS
 CN 2-Phenanthreneacrylic acid, 8-carboxy-4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-4b,8-dimethyl- β -phenyl-, 2-ethyl 8-methyl ester (6CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
 AB Indan (I) or I-contg. hydrocarbon mixts. were catalytically dehydrogenated at 550-670° in the presence of oxides of W, Mo, or Mn. or their mixts. and of steam to give indene (II). Thus, 50 cc. I and 75 cc. H2O was passed as vapor during 2 hrs. through a heated quartz tube (600-50°) containing 230 cc. 1:1 MnO2-MoO3 on pumice to give a product containing 75% II.

AN 1961:87415 CAPLUS Full-text

DN 55:87415

OREF 55:16506b-c

TI Indene

IN Franck, Heinz Gerhard; Grigoleit, Georg

PA Gesellschaft fur Teerverwertung m. b. H.

DT Patent

LA Unavailable

FAN.CNT 1

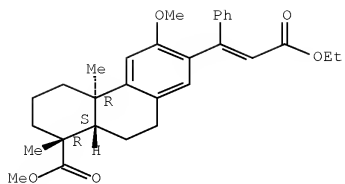
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 1074578		19600204	DE	
IT	124422-36-2				

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 124422-36-2 CAPLUS

CN 2-Phenanthreneacrylic acid, 8-carboxy-4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-4b,8-dimethyl- β -phenyl-, 2-ethyl 8-methyl ester (6CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
66.35	244.92

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-8.00	-8.00

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STN INTERNATIONAL LOGOFF AT 18:04:48 ON 07 APR 2008